L-Valine, N-(2,5-ditrifluoromethylbenzoyl)-, isohexyl ester

Inchi: InChI=1S/C20H25F6NO3/c1-11(2)6-5-9-30-18(29)16(12(3)4)27-17(28)14-10-13(19(21,22

InchiKey: UCIXFVGHQYSETG-UHFFFAOYSA-N

Formula: C20H25F6NO3

SMILES: CC(C)CCCOC(=O)C(NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F)C(C)C

Mol. weight [g/mol]: 441.41

Physical Properties

Property code	Value	Unit	Source
gf	-1233.28	kJ/mol	Joback Method
hf	-1756.45	kJ/mol	Joback Method
hfus	43.39	kJ/mol	Joback Method
hvap	77.39	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	5.458		Crippen Method
mcvol	298.510	ml/mol	McGowan Method
pc	1170.42	kPa	Joback Method
rinpol	2014.00		NIST Webbook
rinpol	2014.00		NIST Webbook
tb	861.81	K	Joback Method
tc	1058.39	K	Joback Method
tf	504.75	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	954.24	J/mol×K	861.81	Joback Method
cpg	968.26	J/mol×K	894.57	Joback Method
cpg	981.29	J/mol×K	927.34	Joback Method
cpg	993.38	J/mol×K	960.10	Joback Method
cpg	1004.61	J/mol×K	992.86	Joback Method
cpg	1015.03	J/mol×K	1025.63	Joback Method
cpg	1024.73	J/mol×K	1058.39	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346571&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume